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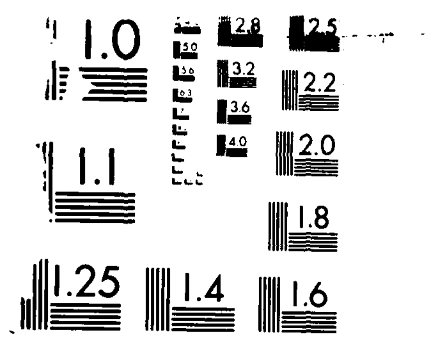

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SECOND ANNUAL PROGRESS REPORT
ON

"NUMERICAL SIMULATION OF TURBULENT FLAMES USING VORTEX METHODS"

AFOSR-84-0356

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SUMMARY

Vortex methods are developed and incorporated in a numerical simulation of turbulent reacting flow, and applied to study the propagation and stability of turbulent flames in different geometrical configurations. At high Damkohler number, a dynamic thin flame model is used, while for slower reactions, the vortex scheme is extended to solve the energy and species equations with finite rate chemical reaction in a Lagrangian particle form. Results have been obtained for a confined mixing layer, a recirculating flow over a rearward-facing step, and a confined shallow cavity. Detailed analyses have been performed to validate the numerical schemes and to study the structure and stability of these flows. The scheme has been extended to three dimension flow and an investigation of the transition to turbulence in an axisymmetric shear layer has been initiated. Currently, the combustion algorithm are being linked to the vortex simulation to predict the interaction between the turbulent field and the burning process. The report includes only new results that have not been published, and a list of the publications that describe previous work.

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Vortex methods are developed and incorporated in a numerical simulation of turbulent reacting flow, and applied to study the propagation and stability of turbulent flames in different geometrical configurations. At high Damkohler number, a dynamic thin flame model is used, while for slower reactions, the vortex scheme is extended to solve the energy and species equations with finite rate chemical reaction in a Lagrangian particle form. Results have been obtained for a confined mixing layer, a recirculating flow over a rearward facing step, and a confined shallow cavity. Detailed analyses have been performed to validate the numerical schemes and to study the structure and stability of these flows. The scheme has been extended to three dimension flow and an investigation of the transition to turbulence in an axisymmetric shear layer has been initiated. Currently, the combustion algorithms are being linked to the vortex simulation to predict the interaction between the turbulent field and the burning process.

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OBJECTIVES:

The goal of the research program is to develop vortex methods for ~~the~~ numerical simulation of multi-dimensional, time-dependent turbulent chemically-reacting flows with high temporal and spatial accuracy. Of particular interest is turbulent shear flows associated with the propagation of turbulent flames in combustion systems. In particular:

(1) Constructing a two-dimensional solution for a confined mixing layer, a recirculating flow, and a cavity flow, and comparing the numerical results with experimental data;

(2) Establishing the limits of application of two-dimensional models for shear flow at high Reynolds number;

(3) Extending the numerical scheme to account for three-dimensional phenomena by modifying the two-dimensional vortex method to include stretching and tilting of vorticity;

(4) Incorporating the thin flame model into the turbulent flow solution and comparing the results with the experimental data;

(5) Defining the mechanism and range of stability of turbulent premixed flames in terms of the relevant physical parameters;

(6) Developing a novel scheme to compute turbulent flames with finite rate chemical reaction under turbulent conditions.

PERSONNEL

Three graduate students have completed their master theses under the sponsorship of this program. Their names and thesis titles are listed at the end of the report. Currently the following graduate students are continuing their doctorate work under the partial of full support of this project:

(1) Ghassem Heidarinejad

(2) Omar Knio

(3) Anantha Krishnan

(4) Habib Najm

(5) Luis-Fillipe Martins

A part-time post-doctoral fellow, Dr. Hany F. Aly, joined our research activities during the period of 1985-1986 to work on the three dimensional vortex simulation and establish a link with the new supercomputer at the John Von Neunamm Center.

EQUIPMENT

To meet the computational needs of this work, we have added the following facilities to a VAX 11/750 with 5 Mb memory and a FP 75, and a MicroVAX II cpu:

(1) An array processor MAP-6420.

(2) Two MicroVAX II workstations.

(3) A local area network.

(4) Communication capability for interaction with a supercomputer.

All the results that we have obtained during the last two years have been obtained using this in-house facilities.

WORK STATUS:

The research program has been divided into four subprojects. A brief description of each project, its current status and the plan for future progress is summarized in the following.

I VORTEX SIMUALTION OF A CHEMICALLY REACTING SHEAR LAYER

(1) Non-Reacting Shear Layer: Vortex simulation of a confined shear layer is used to study the properties of large-scale structures, and to investigate the effect of applying upstream forcing on the dynamics of the eddies and the entrainment of irrotational fluid into the mixing zone. The study of a forced shear layer is motivated by the desire: (1) to improve the understanding of the basic mechanisms in a free shear layer, such as rollup, pairing, the source of subharmonic perturbations, the distribution of energy among and contribution of the large structure dynamics to the velocity statistics, and entrainment; and, (2) to investigate the possibility of actively controlling the rates of mixing. The numerical scheme is constructed to preserve high Reynolds number effects without resorting to turbulence modeling, and to represent accurately the geometry of the channel by satisfying exactly the no-flow condition on the walls.

A large body of experimental data for spatially-developing layers have revealed a number of important features of this flow. Moreover, numerical studies of temporally-growing layer at low Reynolds number have attempted to provide interpretation to these results. However, a temporal simulation does not allow the effect of the velocity ratio or the divergence of the flow to influence the instability, and spatially-growing modes cannot be predicted from a temporal analysis. An accurate numerical study of a forced spatially-developing layer at high Reynolds number is, thus, needed to

address some of these issues. Contrary to previous temporal calculations, no eignfunctions are used to excite the flow, and the sequence of event is produced by perturbations naturally present in the simulation. Results of the forced layer calculations are used to check on the accuracy of the numerical scheme and, meanwhile, elucidating the dynamics of the flow even without forcing.

Results indicate that an unforced layer, when subjected to random perturbations, rolls up at the most unstable frequency which is predicted from the linear stability analysis, and that the rollup eddies equilibrate at a Strouhal number of almost twice the value for the most unstable condition. This duality of the most unstable and the neutrally stable values of the Strouhal number furnishes the ground to explain subsequent pairings and the apparent self-similarity of the unforced layer. Due to the divergence of the spatially-growing layer and the strong non-linearity which accompanies the later stages of rollup, the amplification rate of the latter is smaller than the values predicted from the solution of the Rayleigh equation for a parallel flow. Thus, the comparison with the linear theory must not be attempted beyond the initial stages of rollup where the governing mechanism is clearly produced by a spatially-growing Kelvin-Helmholtz instability waves. Within the range of Reynolds number used in the viscous cases, $R = 40 - \infty$ based on the momentum thickness, the effect of diffusion on the rollup process is negligible.

We find that a forced layer produces eddies at the same value of the Strouhal number, which represents the neutrally stable mode of the layer. The latter explains the strong stability of these resonant eddies, which is manifested by the absence of pairing within this phase of development. Initially, the rollup eddies are formed at the harmonic of the forcing

frequency closest to the most unstable mode of a free shear layer. Immediately after, they are captured by the wave produced by the forcing mechanism, and the non-linear interaction between the two waves results in the formation of the resonant eddy. This interaction is either an accelerated pairing of two eddies or a group merging of more than two eddies, depending on the forcing frequency. Thus, forcing organizes the shear layer structure so that a resonant eddy forms earlier than the eddy with the same frequency would form in an unforced layer. For several wavelengths downstream, resonant eddies do not pair, instead they form a train of identical elliptical structures. A small amplitude perturbation, of the size of 1% of the incoming fast stream, is found to be sufficient to produce this effect. These eddies move downstream at the average flow speed. If the background noise in the free stream is high, higher amplitude forcing is necessary.

Large eddies start to pair when the local subharmonic perturbation amplifies to a maximum. This is observed most clearly in a forced layer since forcing quantizes the energy spactrum to amplitudes higher than the background noise and organizes the spatial growth of the layer. The perturbation is produced by the action of: (1) the relative displacement of the centers of neighboring eddies by the divergence of the main stream due to the velocity difference; and (2) the growth of the large structures downstream due to pairing. In a forced layer, the formation of identical resonant eddies delays pairing by forming a train of identical eddies, hence removing temporarily the two catalysts of the subharmonic perturbation. Forcing is only effective on eddies with passage frequencies equal to or higher than the forcing frequency. Beyond that stage, the layer acts as an unforced layer. The length of this region depends on the forcing amplitude.

Velocity statistics of a forced layer shows that the sign of Reynolds stresses depends on the relative position of the emerging eddies or the orientation of the newly-formed large eddies. In an unforced layer, eddy pairing occurs soon after the formation of two eddies of the same frequency, and the computed Reynolds stress is positive across the layer everywhere downstream of the splitter plate. Thus, the prevailing interaction between the mean stream and the large eddies is that of positive energy transfer into the large eddies. On the other hand, forcing impairs pairings of the resonant eddies, and zones of negative shear stresses arise, reaching a maximum immediately following pairing. Withing this range, large eddies are feeding energy back into the mean flow and "counter gradient diffusion" is observed. This dynamical property, which emphasizes the role of large scale structures in turbulent flow, cannot be implemented in gradient-diffusion type turbulence model where the sign of the turbulent stresses is dependent on the gradient of the average velocity.

Results of this work have been published in Ng and Ghoniem (1985), Ghoniem and Ng (1986).

<u>(2) Entrainment and Mixing in a Thermally-Stratified Shear Layer</u>: Our results indicate that in a homogeneous natural, unforced - layer, most of the entrainment of irrotational fluid from the free streams takes place immediately after pairing when an eddy engulfs the newly formed braids along with the surrounding fluid. Thus, the process is controlled by the flow into and within the braids instead of the field within the cores. The strong strain field within the braids, which is established by the large rotating cores, is capable of pulling fluid from outside the original shear layer into the mixing zones of the large cores. Entrainment into the mixing zone is therefore biased towards the high speed stream where more fluid is

forced into the large structures. In the forced layer, accelerated pairings at the initial stages increases entrainment, while inhibiting pairing reverses the trend and the layer maintains a constant thickness until it resumes its natural pairings again.

To simulate and study the entrainment and mixing in a heterogenous layer, i.e. a layer formed of streams initially at different temperatures, or streams initially carrying different species such as fuel and oxidizer, we have constructed a new computational scheme which we call "Moving Gradient Method." The scheme is based on the use of Lagrangian computational elements to transport the gradients of a scalar, energy or species concentration, in a way similar to the vorticity transport using vortex elements in vortex simulation of Navier-Stokes equations. The same computational particles used to carry the vortex elements are actually employed to transport the scalar, or scalars gradients, and hence no extra computational labor is wasted in the transport process. The local value of the temperature, or the scalar concentration, is obtained by intergating over the gradient elements, which involves a summation over the fields induced by all the gradient elements. The scheme is fully Lagrangian and grid-free, thus the numerical diffusion is minimized and the computational elements are moved to capture the large gradiends in the flow field rendering the computational automatically adaptive in time and space. All the tools developed to perform accurate vortex simulation can be extended to obtain accurate solutions of the energy and species equations at high Reynolds numbers and computations of the temperature field in a mixing process can be obtained.

The procedure starts by discretizing the initial temperature gradient (heat flux) among the particles carrying the vortex elements and assigning a

local strength to each element such that the accumulative value of the gradient at each point is the same as the given value. The transport is then implemented by moving these elements at the local value of the velocity. During this step, the strength of the elements remains constant. A set of ordinary differential equations is then integrated to compute the new strength of the gradient elements after they have been transported to their new locations. This is necessary because while the total energy is conserved, the local temperature gradient is changing by the change in the streamline pattern with time. It is important to mention here that elements that are exposed to large strain fields must be divided into two, or more, to maintain the accuracy of the calculation at the desirable level. The total strength of the elements should remain the same during this process, however, and care must be exercised in interpolating the strength of an element between several elements. If two elements move very close to each other, they are combined to form a new element that aquires their total strength and is located at the center of mass of the original elements.

Preliminary results of the calculation of a temporally growing thermally stratified shear layer are shown in Figures 1, 2, 3 and 4. In the first set of results we show the evolution of a turbulent eddy by plotting the location and velocity of all the vortex elements used in the computations. Note the generation of very sharp velocity gradients where the braids of the eddy are becoming extremely thin due to the very strong strain field that exists between neighboring cores. Up to our knowlege, the only way to capture this gradient is using the scheme that we are developing here. Previous computations which employed a grid to discretize the equations had to be performed at very low Reynolds numbers and to be stopped before the stage when the braids became thin. Near the center of the eddy,

intense mixing between the fluid elements entrained from the free streams is observed. Mixing is also enhanced by the strong stretching of the layer at this point. Figure 2 shows a comparison between our computations and experimental results showing the different stages of roll up of a shear layer. Figure 3 shows the formation of large eddies and their subsequent pairings when a subharmonic perturbation is imposed.

Figure 4 shows the temperature distribution across the layer at different stages of development, indicating the generation of sharp temperature gradients withing the cores during the rollup process, a phenomenon that has been observed in careful experimental studies. Later on, the homogenization of the fluid within the core of each eddy is achieved. These results compare favourably with the experimental data of Konrad. Details of the scheme and the results of the rollup of the shear layer will appear in a forthcoming publication (Ghoniem, Hiedarinejad, and Krichnan 1986).

In the next phase of the project the scheme will be extended to include the effect of molecular diffusion by expanding the core of the gradient elements at a rate proportional to the diffusivity. We are also planning to solve for the spatially growing layer, as well as to implement the scheme in different flow configurations such as the recirculating flow.

(3) Chemically Reacting Shear Layer: The first attempt to study a turbulent diffusion flame will be presented in the paper by Givi and Ghoniem (1987). A rudimentary model of combustion is used in this article to emphasize the power of using a Lagrangian scheme in the comuputations of chemical reactions. However, density effects could not be modeled in these computations and and a more powerful technique was developed.

For that purpose, the moving gradient element method was extended to simulate a chemical reaction between the two streams by including the chemical source term in the energy equation, the density gradient in the continuity equation and the non-baroclinic vorticity production term in the vorticity transport equation. The scheme lends itself naturally to this case, since the energy equation in terms of the heat fluxes must be integrated to compute the new strength of the elements. The strength of the elements change due to transport as well as reaction simultanuously and in the same step of integration. Chemical reaction occurs within each particle, and hence it is performed in Lagrangian coordinates.

The volumetric expansion associated with the conversion of reactant into products interferes with the dynamics in two ways: (1) it adds an irrotational velocity field that acts to expand the reaction zone; and (2) it modifies the vorticity field according to the pressure-density interaction across the reaction zone. Both effects are included in the numerical model by allowing vortex elements to act as volumetric sources and by changing the circulation of each element as it moves through the flame zone, respectively. Thus, non-baroclinic effects due to combustion at low Mach number are implemented in the computations without artificial modeling.

Work is underway to study the following problems:

(1) the stability of a turbulent premixed flame forming between a reactants and a products streams moving at different velocities. The reaction rate takes an Arrhenius form with a moderately high, but finite, activation energy, while the temperature ratio is in the range of 5-8;

(2) the blow-off of the flame at low equivalence ratios due to the strong strain field within the braid sections, and in particular, the effect of Lewis number on the extinction of the flame.

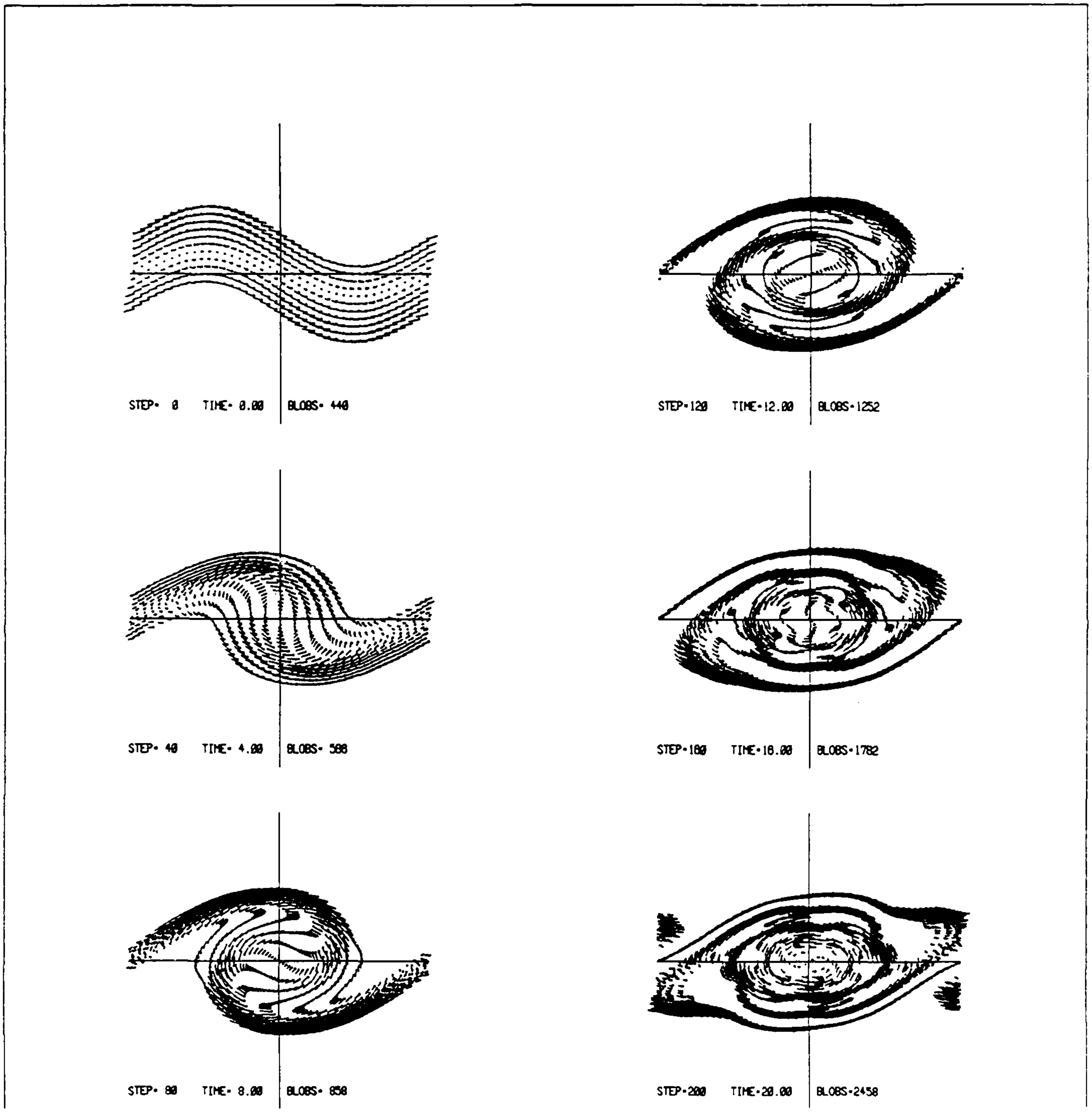
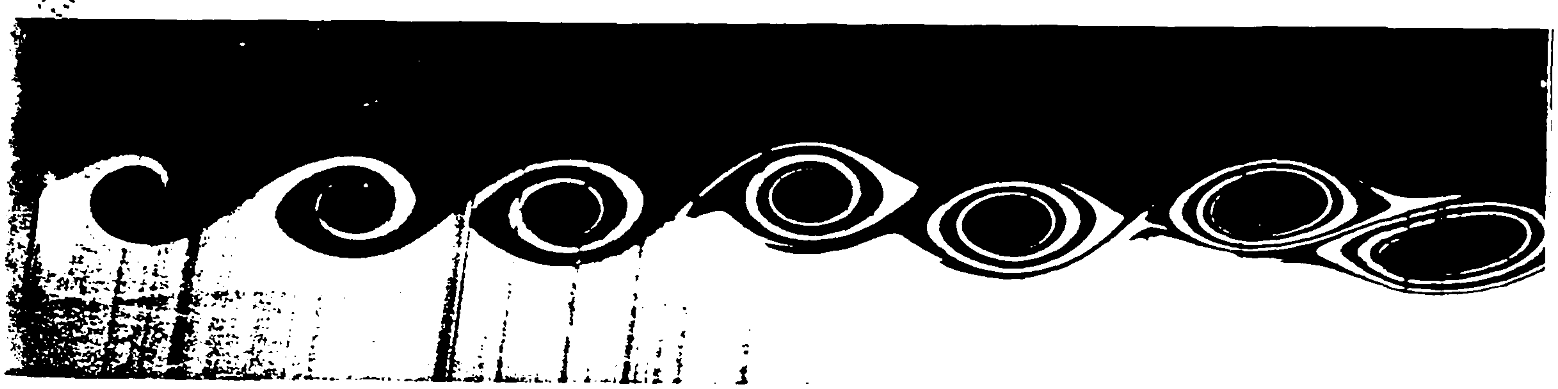
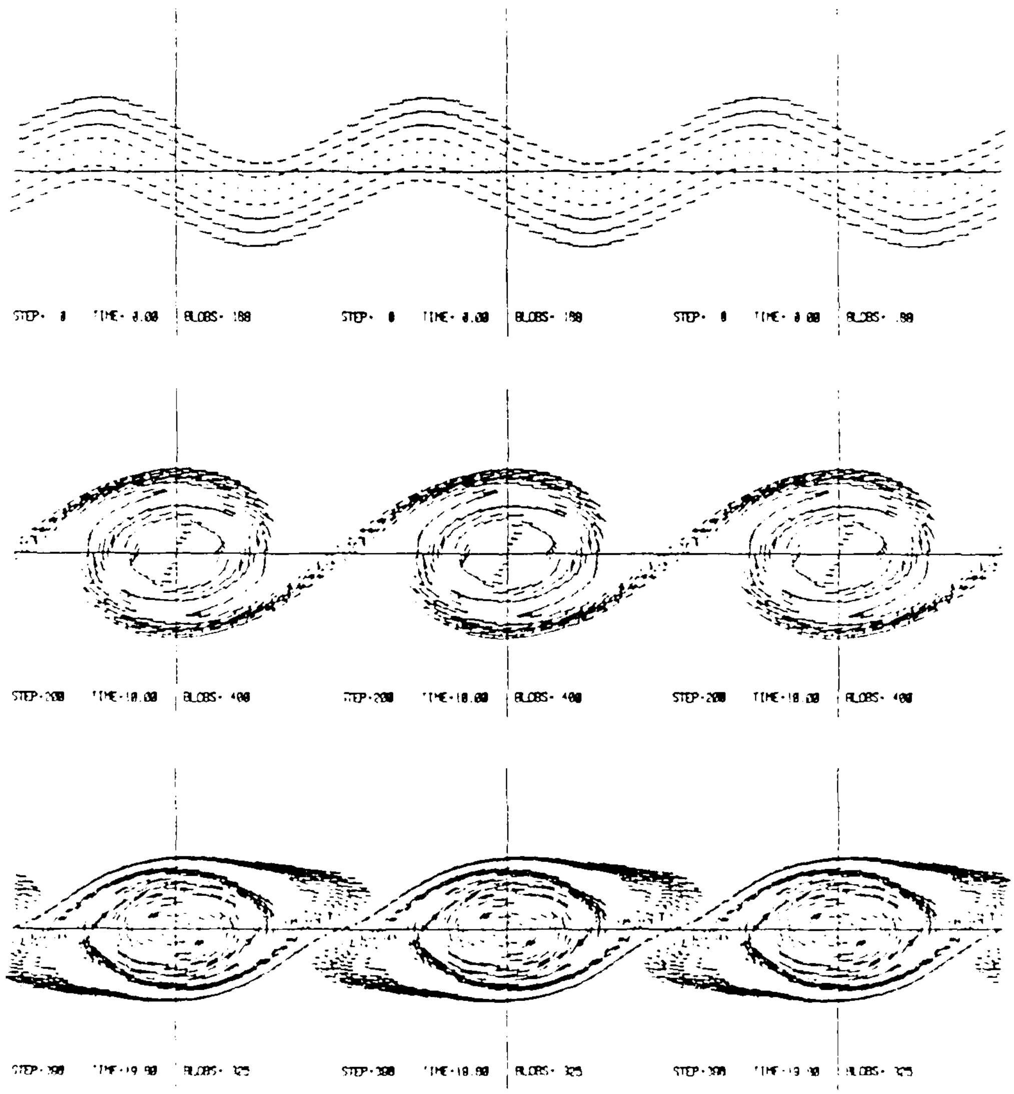


Figure 1 The roll-up of an unstable shear layer perturbed at the linearly most amplified wavelength. The circles depict all the vortex elements used in the computations, and the lines indicate their instantaneous velocity vectors. The last figure show the stage when the layer attains dynamical equilibrium and the envelope ceases to rotate.





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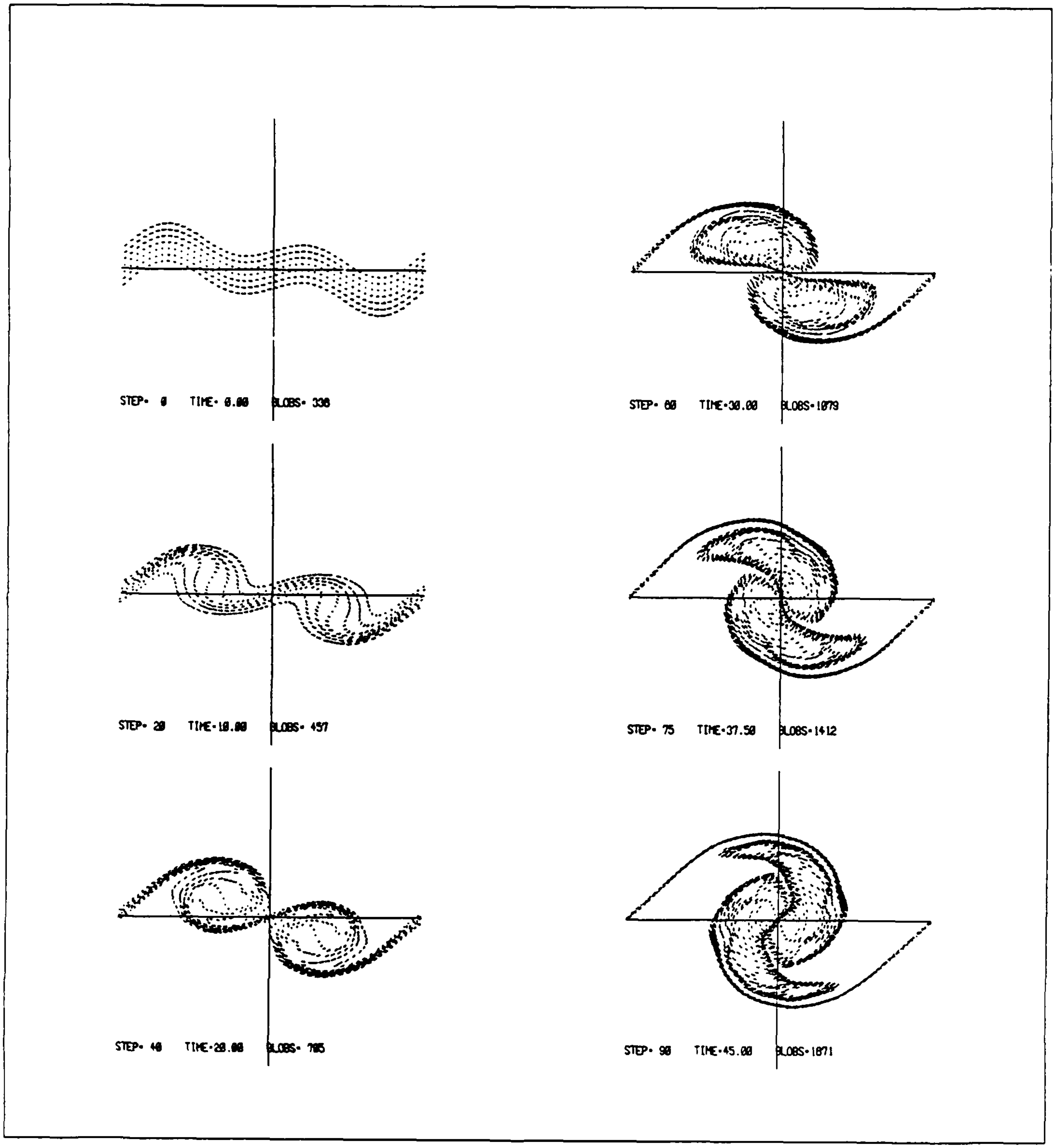


Figure 3 Pairing of two large eddies, formed by roll up and forced to pair under the influence of the subharmonic perturbation.

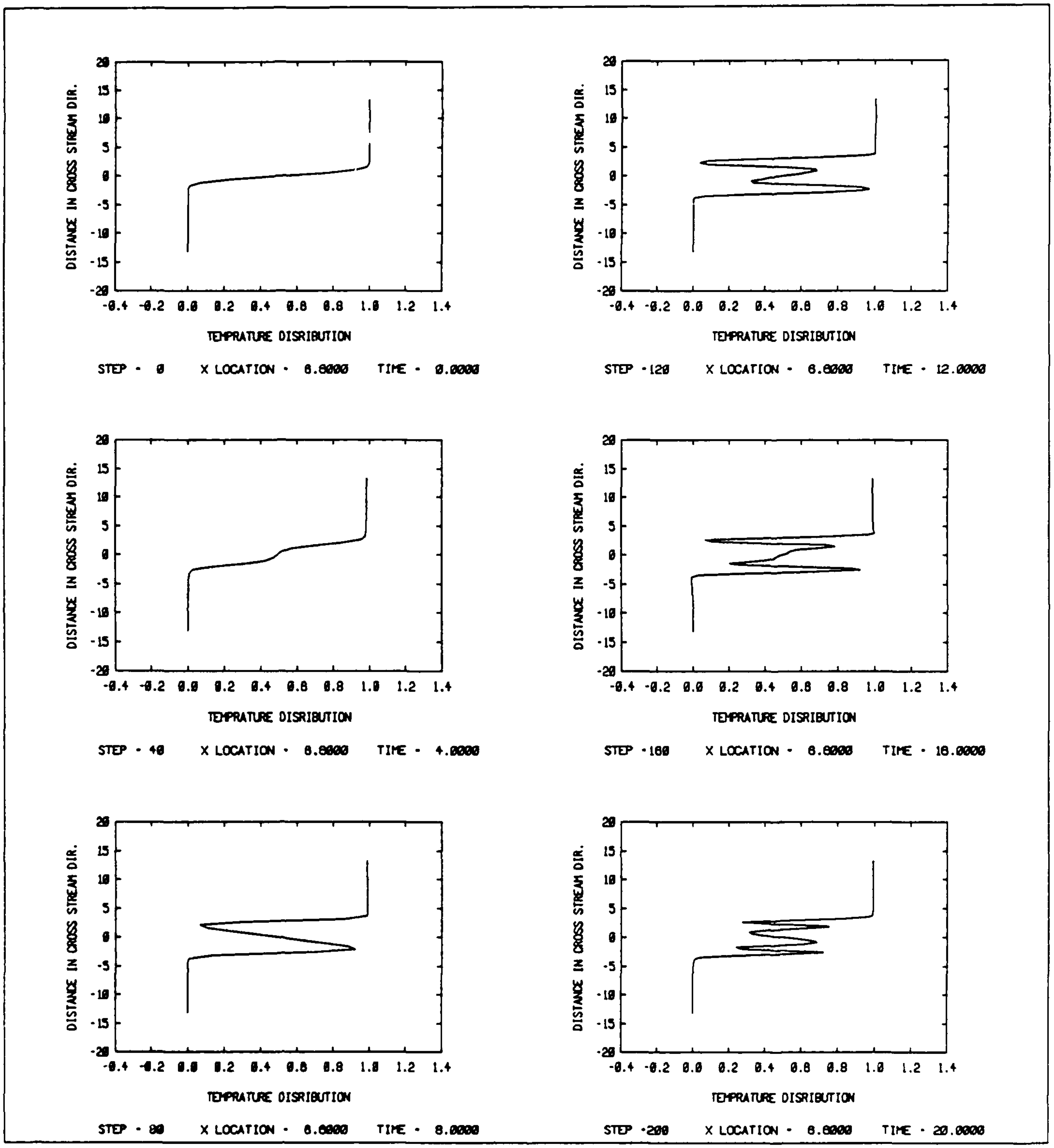


Figure 4 Temperature distribution across the center of the large eddy, computed using the moving gradient algorithm, and showing the effect of the roll up on the formation of tongues of hot fluid in the cold stream and vice verca, as shown experimentaly.

II NUMERICAL STUDY OF COMBUSTION INSTABILITY IN DUMP CONFIGURATION

The goal of this work is to identify the mechanism leading to the combustion instability observed in dump configuration at equivalence ratios close to unity. The instability manifests itself in the formation of high amplitude pressure oscillation, accompanied by the periodic motion of the flame front from a location upstream of the anchoring point down to the reattachment point of the recirculation zone. The phenomenon is perfectly periodic and self-sustained, which led to the belief that it is acoustic in nature and to the use of the Rayleigh criterion of flame-sound wave interaction in the interpretation of experimental data. However recent experimental and numerical studies of recirculating flows have revealed that non-reacting flow at moderate Reynolds numbers possesses periodic oscillations associated with the formation of well-organized large scale vortex structures in the shear layer. In this work, we use vortex simulation to study this flow and quantify the dominant frequencies. Results are then used to identify the mechanism leading to the formation and sustenance of the instability.

The scheme we employ has been used in the study of recirculating flow over a rearward-facing step at intermediate and at high Reynolds numbers. Results of the first case were utilized to investigate the accuracy of the scheme, and to study the change of the structure of the recirculation zone as the Reynolds number increases. Results of the second case revealed the onset of unsteadiness associated with the formation of large eddies and their interaction downstream.

(1) Vortex Simulations at intermediate Reynolds numbers: Computations of a recirculating flow downstream a rearward-facing step in a channel, at values of Reynolds number for which two-dimensional, steady flow is

experimentally observed, were performed using the random vortex method. Our choice of the test cases and the regime of Reynolds number, while mandated by the availability of experimental results for comparison, represent a problem that is fundamentally challenging and practically important. Converged results, obtained by successive stepwise refinement of the numerical parameters, showed good agreement with the experimental results. The behavior of the error suggests that the variation of the number of vortex elements as a function of the circulation of each element can be used to judge the accuracy of the computed solution. The criterion depends on the fact that, within a specified computational domain, the total circulation in the field should be invariant to the strength of a computational vortex element.

The numerical solutions of steady problems show that the number of elements used in the simulation has the strongest influence on the accuracy. Using a small number of elements to discretize the vorticity field produces errors that reduce the reattachment length for the recirculating flow. In this computations, when the number of vortex elements exceeded a critical value, the initial separation between vortex sheets and the time step, if chosen small enough, were of secondary importance. The number of vortex elements required to achieve accurate results depended weakly on the Reynolds number. Averaging over ten time steps removes the statistical error and yielded essentially smooth profiles that compared favorably with the analytical solution of a steady channel flow. For the recirculating flow, as the Reynolds number increased, averaging over an increasing number of time steps was necessary to compute a steady-state solution.

Results of this study have appeared in Ghoniem and Gagnon (1986).

(2) Vortex Simulation at High Reynolds Numbers: Results of the numerical simulation of the flow behind a rearward-facing step demonstrate that the flow becomes unsteady beyond the viscous range of small Reynolds number, and that the underlying mechanism in the evolution of vortex structures is periodic. By controlling numerical diffusion as the Reynolds number increases, small eddy shedding is observed at the step and along the wall boundary layers, accomapnied by a change in the flow dynamics. The computations covered a wide range of Reynolds numbers, 50 to 5000, and were obtained using the random vortex method. While the calculations apply to a strictly two-dimensional flow, results show the transition of the flow dynamics from viscous into laminar flow at low Reynolds numbers, up to transitional and turbulent flow at high Reynolds numbers. Both the variation of the flow structure and the velocity statistics were used to identify different flow regimes. The following observations are emphasized:

(1) At very low Reynolds number, the recirculation zone is small and stationary. Viscous forces dominate the flow field;

(2) As the Reynolds number increases, and under very weak forcing via numerical noise, an eddy detaches from the shear layer when its size reaches a critical value. As this eddy moves downstream, another eddy forms. The flow is laminar and stable;

(3) At moderate Reynolds number, the oscillation of the recirculation bubble becomes stronger and the separating shear layer rolls up into small eddies that grow by pairing. Reattachment length reaches a maximum and the flow starts to separate from the opposite wall;

(4) At high Reynolds numbers, the rate of growth of the separating shear layer increases. Close to the step, small eddies form at the point of separation and along the wall, with a counter-rotating eddy at the lower corner. A separation bubble forms on the opposite wall.

(5) A corner vortex appears between the recirculation zone and the lower corner at $R \geq 500$, and remains for at higher Reynolds numbers;

(6) The rate of growth of the separating shear layer increases at higher Reynolds number.

The numerical results reveal the large-scale structure of the recirculation zone at high Reynolds numbers. This structure forms as a manifestation of an intrinsic flow instability that promotes the vorticity in the separating shear layer to roll up. The existence of vortex structures in both laminar and turbulent free shear layers has been well established experimentally and numerically. With the formation of a well-defined set of large eddies, one frequency dominates the flow. This suggests that proper averaging to evaluate flow properties and their moments should correlate with this frequency. Numerically, that may correspond to a moving time/space window laid over the data, whose frequency corresponds to eddy motion. We are currently exploring the design of such numerical tools for use in the study of the evolution of vortex structures.

At low Reynolds number the recirculation zone is formed of a small stationary eddy at the corner of the step. As the Reynolds number increases, the eddy grows by entraining more vortical fluid then detaches and another eddy forms. The separating shear layer becomes unstable at higher Reynolds number, causing small eddy shedding, and forming a set of interacting vortices that extends the recirculation zone further downstream. Eddy pairing and wall interactions dominate the flow for Reynolds numbers in the early turbulent range, causing the recirculation zone to become shorter and more stable.

Results of this study have been published in Ghoniem and Sethian (1985) and Sethian and Ghoniem (1986).

Similar change in the structure of the recirculation zone and the separating shear layer was observed in computations for a flow over a shallow cavity, to be named a dump configuration in the next section, for the same range of Reynolds number. This result indicates that this transitional instability is an intrinsic phenomenon to recirculating flows and is alomost independent of the system itself (Najm and Ghoniem 1986).

(3) Simulation of a Dump Configuration: Results of the numerical simulations of a flow over a long shallow cavity, obtained for inlet flow Reynolds number 2000 are shown in Figures 5, 6 and 7 in the form of the instantaneous location and velocity of the vortex elements, the instantaneous streamlines and the spectrum of the oscillations, respectively. Similar results were obtained for higher Reynolds numbers of 5000 and 10000. They indicate that the referred peaks correspond to the passage frequencies of eddies originating at the upstream cavity edge and their subharmonics. The frequency of shedding, $\Omega 1$, is significant mainly near the upstream edge where the shear layer rolls up according to its most unstable mode. The corresponding Strouhal number based on the momentum thickness of the boundary layer, the mean velocity of the incoming flow and the frequency is 0.016, in agreement with the experimental results for double expansion. The eddies pair as they travel downstream, thus providing a subharmonic frequency $\Omega 2 = \Omega 1/2$. Depending on the length of the cavity, these eddies may or may not have the chance to undergo another pairing before they reach the downstream end of the cavity. For the case where this does occur (cavity length/depth $L/D = 4.0$), the final generation of eddies are twice the cavity depth in diameter and their collision with the downstream edge causes a global flapping of the shear layer at a frequency $\Omega 3 = \Omega 1/4$. The dynamics can be seen in the time sequence of pictures of the

flow shown in Figure 5. The dynamics can further be observed by following the streamline plots of the flowfield in the cavity, Figure 6. The spectral distribution of the vertical velocity fluctuations in the shear layer above the cavity at several locations in the streamwise direction is shown in Figure 7 (Ghoniem and Najm 1986).

The flapping of the outer edge of the shear layer, which we observe in the numerical results at the lowest observable subharmonic frequency is in agreement with the experimental results. This event has been referred to as the "preferred mode of jet oscillation", to distinguish it from the shear layer mode at separation. The numerical results indicate that this flapping is a manifestation of the passage of the last generation of merged eddies and their destruction as they collide with the downstream step. Therefore, this is not an independent phenomenon, and it is a consequence of the essential dynamics of the shear layer which is dominated by eddy pairing. The similarity between the flapping of the outer edge of the shear layer and that of premixed flames in a similar geometrical configurations during the unstable mode is the key to explaining the latter. However, before doing that, two facts should be emphasized: (1) for turbulent flames stabilized on shear layers, and when the burning velocity is much less than the typical flow velocity, the front exists on the outer edges of the vorticity layer and the motion of the flame follows closely the motion of the layer; and, (2) three modes of instability have been observed experimentally, humming, buzzing and flapping (flashback), corresponding to three distinct frequencies which were also observed in the spectrum of the stable mode. These three modes correspond to the shear layer frequencies computed above.

Since the shear layer possesses three distinct frequencies, the flow can be tuned so that one frequency dominates and the other two frequencies

are supressed. This may be achieved by adding a small oscillatory component to the incoming velocity, the upstream pressure or the rate of heat release. The latter is naturally present in our case since the flame length, which is determined by the demarcation line between the vortex and the non-vortex fluid, changes its length at the dominant frequency. Thus, the oscillation in the heat release rate can tune the shear layer, which in turn sustains the oscillation in the heat release. This hypothesis is being currently investigated numerically by combining a heat release model that was independently developed and tested using experimental data on constant volume combustion (discussed in the next section) and the vortex simulation. This study will show how heat release can amplify the instability of the shear layer and tune a particular frequency so that a single eddy dominates the observable dynamics.

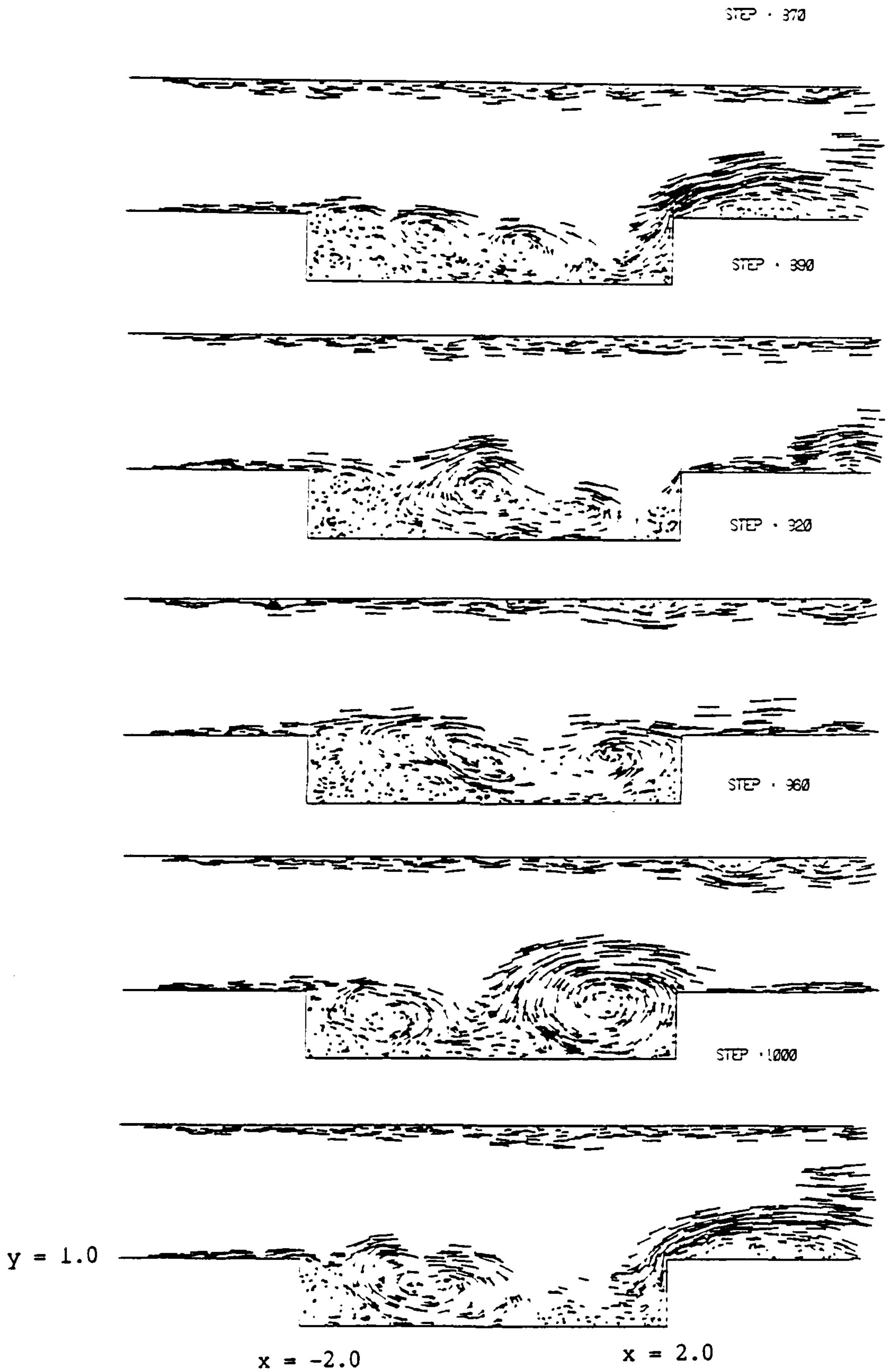


Figure 1 : Instantaneous location and velocity of vortex elements for a sequence of time steps. Two consecutive pairings occur, resulting in a large eddy that is destroyed upon collision with the downstream cavity edge.

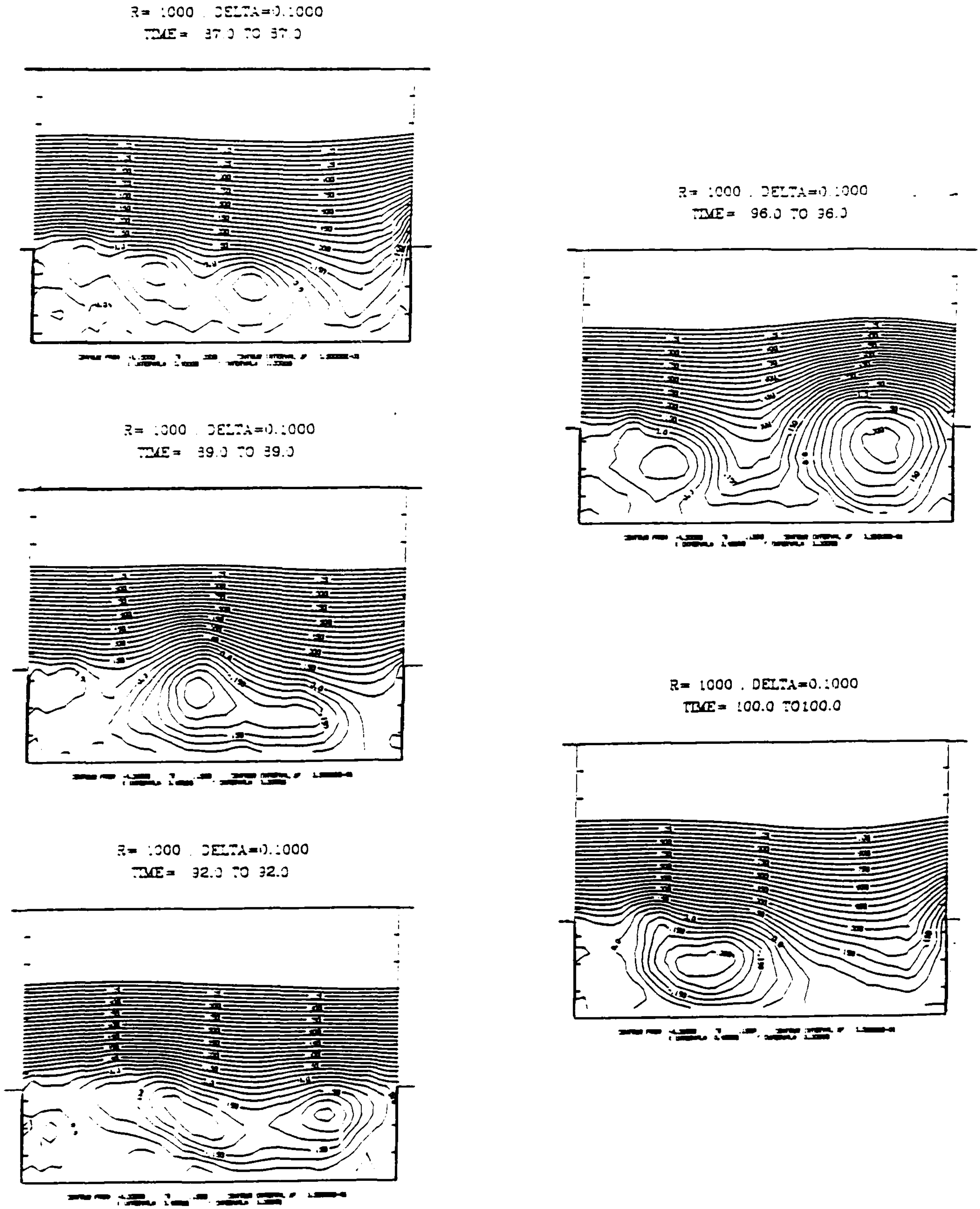
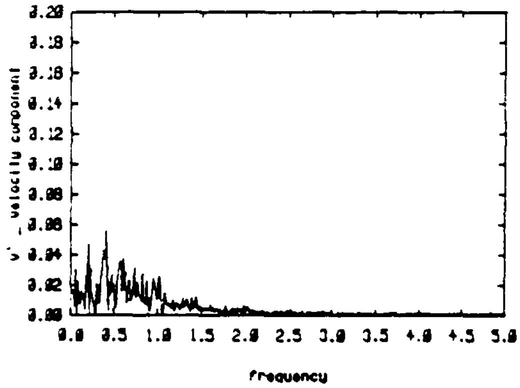
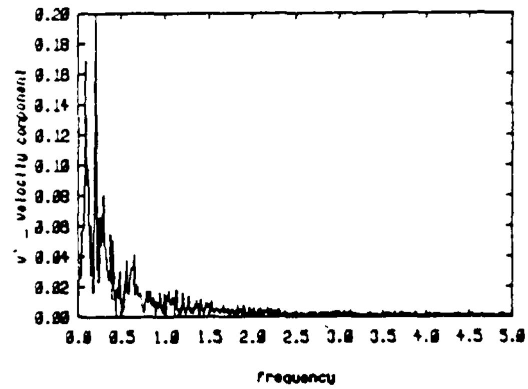


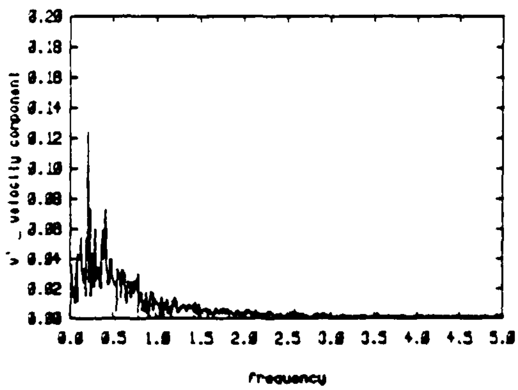
Figure 2 : Time sequence of plots showing the instantaneous streamlines inside the cavity corresponding to the frames in Figure 1. The two pairings, as well as the resulting elevation and depression of the shear layer due to the passage of the final large eddy, are clearly seen.



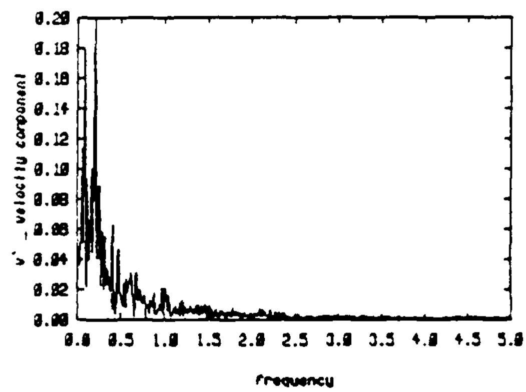
x = −1.8 y = 1.0



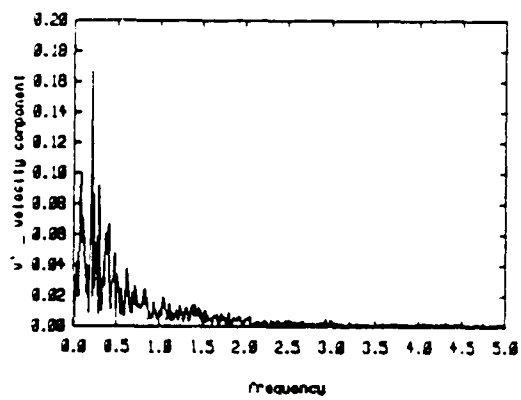
x = 0.0 y = 1.0



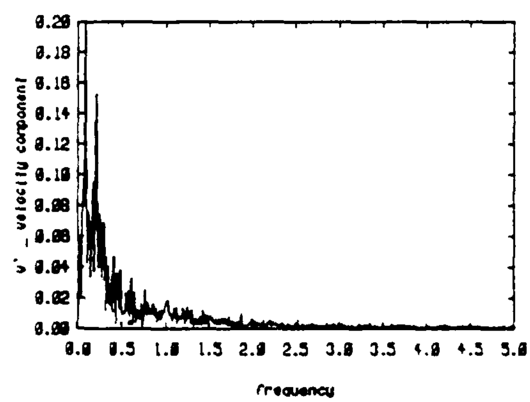
x = −1.2 y = 1.0



x = 0.8 y = 1.0



x = −0.8 y = 1.0



x = 1.2 y = 1.0

Figure 3: Velocity fluctuation spectra for the same flow case depicted in Figure 1 taken at six different locations along the shear layer over the cavity. The highest peak occurs at approximately : 0.4, 0.2 and 0.1 dimensionless frequency, depending on the streamwise location.

III DYNAMICS OF TURBULENT PREMIXED FLAMES

In this work, a computational model for the calculation of premixed flame propagation is developed. The purpose is to construct a combustion model that an be linked to the vortex simulation of recirculating flow in the computation of the dump combustor instability. The model utilizes recent theoretical results on flame stability, namely the dependence of the normal burning velocity on the curvature of the flame front, and can be further enhanced to account for the effect of flow curvature on the burning velocity. As a validation case, computations were performed for combustion in two dimensional circular and rectangular chambers, and results were used to investigate the accuracy of the model by comparison to experimental data. The evolution and stability of the front were examined, and the contribution of molecular processes, the large scale flame curvature and the interaction between the flame and its self generated field on the dynamics of the combustion process were analyzed. The effect of large scale eddy motion on the rate of burning waas also analyzed using this scheme.

Results of our study show that accurate modeling of combustion of quiescent premixed gases at high Damkohler numbers inside closed, constant-volume chambers requires the use of numerical schemes that can appropriately capture the dynamics of tne thin flame front. The numerical model should take into account the variation of normal burning velocity with the thermodynamic state of the reacting mixture and with the curvature of the front. When done, results of the computations compare favorably with experimental data on flame geometry and position, and on pressure history. Some deviation was observed due to: (1) departure of the products of combustion from perfect gas behavior; (2) flow stretch effects, which become particularly important in the presence of a turbulent flow field; and, (3)

heat losses across the walls of the enclosure which can alter significantly the thermodynamic state of the reactive mixture if the flame propagate along the walls for an extended period of time. Deviation from perfect gas behavior and heat losses across the enclosure walls can be tackled. The flame curvature algorithm can be used to compute the flow stretch component, since this algorithm yields readily the angle of inclination of the flame with respect to the flow field, and the result can be used to modify the burning velocity. This is particularly important if initial turbulent motion is present at the moment of ignition.

Curvature contributes to the stabilization of flame fronts at two scales. At small scales compared with the flame thickness, heat diffusion improves the stability of the front at large Lewis numbers, as shown analytically by the results of the linear analysis and numerically in this work. At large scales, the following non-linear processes appear to play an important role:

(1)The growth of perturbations along the flame front. This leads to a significant change in the flame geometry and, in turn, a substantial modification of the flame-generated flow field. The distortion in the flow ahead of the front is found to counteract the mechanism of the instability. Unlike heat diffusion which mainly affects small wavelength perturbations, this effect is independent of the wavelength of the perturbation.

(2)The consumption of the concave parts of the front as the flame expands. A sinusoidal perturbation of large amplitude develops as follows: the concave part grows into a deep cusp and the concave part maintains its roundness towards the reactants. As the angle between the two sides of the cusp increases, the concave part becomes flatter while the convex part grows further. Thus, non-linear evolution eventually leads to the smoothing out

of the original perturbation and the development of a curved front with narrow valleys and wide peaks into the reactants. The formation of stable curved flame fronts protruding into the reactants as a limit of the non-linear evolution of the hydrodynamic instability has been predicted before on the basis of pure geometrical considerations.

(3)The expansion of the flame into a curved surface. This leads to the stretch of perturbations as they move along the surface. The stretch of the perturbations increases of the wavelength and hence reduces the rate of growth of the amplitude, rendering curved fronts more stable than planar fronts.

Computational results were used to explain the formation and evolution of tulip flames. The distortion of the flame front and the development of indentations is a consequence of the growth of perturbations by the mechanism of hydrodynamic instability when the value of the Markstein length is small. The formation of the tulip is delayed, or prevented, when the flame is stabilized by a large value of the Markstein length. Thus the outcome of the evolution of the flame depends on the initial conditions since the Markstein length is a strong function of the mixture and the equivalence ratio. Similar behavior was observed for propagation inside a circular and a rectangular chambers, indicating that this mechanism is independent of the geometry of the enclosure and arises as a result of the imbalance between the local flow velocity and the burning velocity.

Results of this study have been published in Ghoniem and Knio (1986) and Knio and Ghoniem (1986).

The code is currently being interfaced with the vortex simulation code to analyze the effect of heat release on the stability of the flow field in a dump combustor configuration.

IV THREE DIMENSIONAL VORTEX SIMULATION

Most shear flows encountered in combustion systems, such as boundary layers, shear layers and jets, start out as two dimensional flows. Two dimensional instabilities, Tollmien-Schlichting for the first and Kelvin-Helmholtz for the second and third case, lead to the formation of large structures whose axes lie normal to the plane of the mean flow. The interaction between these structures and their effect on the combustion process is the subject of the first two projects in this report. The stability of the inviscid two dimensional structures that appear in shear layers and jets to three dimensional perturbations is studied here.

Judging from an abundence of experimental evidence, transition to three dimensional flow is unavoidable at the later stages of development of a shear layer. Moreover, this transition and the generation of three dimensional structures will have a noticeable effect on the mixing process, a situation which has been labelled "mixing transition." The formation of three dimensional secondary vortices around the outer edges of the primary vortices seems to be the mechanism by which local diffusion is enhanced. Mixing, resulting from the diffusion within the large structures, is thus dependent on both the two dimensional dynamics and the formation of these three dimensional vortices. In this work, we are looking for the origin of these vortices and their subsequent interaction with the flow. The objective of this project is, thus, to extend two dimensional vortex methods to three dimensions and use the developed algorithms to study the evolution and structure of turbulent shear flows beyond the two dimensional range.

Vortex methods are natural candidates for the computations of highly concentrated regions of vorticity that evolve rapidly with time since they concentrate computational elements where vorticity is non zero, and track

this vorticity as it moves in the fluid. We have constructed a three-dimensional time-dependent vortex simulation using the vortex-vector element scheme (Ghoniem, Knio and Aly 1986). The scheme is designed to track the evolution of finite core thin vortex tube in terms of finite length vortex vectors in three dimensional space using a combined Biot-Savart velocity calculation and a finite volume method to satisfy the potential boundary condition on the boundaries. Vortex vector elements possess a finite core of vorticity with a distribution that is assigned at the initial stages to model the actual vorticity of the flow field. The accuracy of the calculations can be improved by changing the distribution of vorticity inside the cores and/or using shorter vortex vectors anlog the tubes.

A computer code implementing this method has been developed and tested on our VAX-system using a model for a single vortex filament in an infinite domain or an array of periodic vortex rings. Preliminary results confirm the accuracy and stability of the numerical scheme. For more elaborate physical models which require the use of a large number of vortex tubes, the code has been transferred onto a CYBER 205 supercomputer, and a new vectorized version of the code has been implemented. The vortex-vector element algorithm is easily vectorizable since the computations are explicit and proceed by looking at the interaction between an element and the entire array of elements. Moreover, it can utilize efficiently the parallel structure of supercomputer when available.

Since most shear layers that form in practical devices are axisymmetric, we concentrate on computing flow fields which start out as being axisymmetric. The early stages of development of an axisymmetric shear layer are almost identical to those of a planar layer, i.e., the vorticity layer, which may be called a sleeve or a shell of vorticity, rolls

up into large scale vortex rings due to Kelvin-Helmholtz instability (as shown in Figures 1, 2 and 3). These ring vortices are characterized by a certain core/radius ratio that depends on the shell radius and initial thickness. The stability of these rings to radial perturbation is believed to be responsible for the generation of three dimensional motion and streamwise vortices. A numerical study of the linear and non linear instability of these ring is, thus, an important first step towards understanding the source of the three dimensional motion and its effect of the evolution of the shear layer beyond the two dimensional phase.

We started be applying a small perturbation, of amplitude 0.02 of the ring diameter, to rings with core/radius ratio in the range of 0.1-0.25. The wavelength of the perturbation is determined by the number of sine wave that are fitted around the ring circumference, only an integer wave number (number of waves) can be used. That number ranged from 1 to 25 in this study. We found that for each ring there is a window of instability in the wave number spectrum, outside this window the ring is stable to small perturbation. This window is formed of 1-3 wave numbers. These results are in very good agreement with the conclusions of the linear theory of stability of vortex rings, which was developed by Widnall et al. during the past decade (Phil. Trans. R. Soc. Lond., A287, p. 34, 1977).

Figure 8 shows the evoluation of an unstable vortex ring with core/radius = 0.25. The figure is plotted for every 100 time steps of computations. The initial perturbation is made of n = 6 azimuthal two dimensional sine waves with amplitude 0.02 of the radius, applied in the radial direction, all in the plane of the ring. Starting with n = 1 to 15, we found that this is the only unstable mode of the ring, i.e. for n = 1 to 4, and n = 8 to 15, the waves only travelled along the ring without

amplification. For n = 5 and 7, we noticed a small amplification, followed by no further growth. These values agree with the theory of linear stability of vortex rings of Widnall. For n = 6, the waves grow in three stages; (1) linear stage, shown in Figure 8(a), where the form of the wave remains the same as the initial perturbation while the amplitude grows exponentially. During this stage, the wave crests bend backwards in the streamwise direction and start to stretch forming inverted U-shape streamwise vortices (horse-shoe) out of the original ring; (2) non-linear stage, depicted in Figure 8 (b), where the inverted U-shape vortices stretch out further without changing their basic form; and (3) the last stage, Figure 8(c), where the waves turn around and start moving forward towards the original ring. This stage is associated with strong stretch and the formation of local concentrations of vorticity at the leading edges of the waves. Moreover, some forwad motion is observed, leading to the formation of another set of streamwise vortices that lead the ring.

We are currently compiling data that will help us to understand this interesting instability for rings of different core/radius ratio. Of particular interest is: the rate of growth of the perturbation in various satges, the spectrum of the ring and the associated velocity field, the "fractal" nature of turbulence at the final stages of development, and its effect of the overall flow field. Moreover, for more accurate simulation of the fat ring, i.e. for core/radius more that 0.25, we are developing a scheme for discretizing the physical ring into a number of overlapping computational vortex tube. Finally, the code is also being adapted to study the formation of the ring by perturbing a shell of vorticity in the streamwise vorticity and watching its roll up.

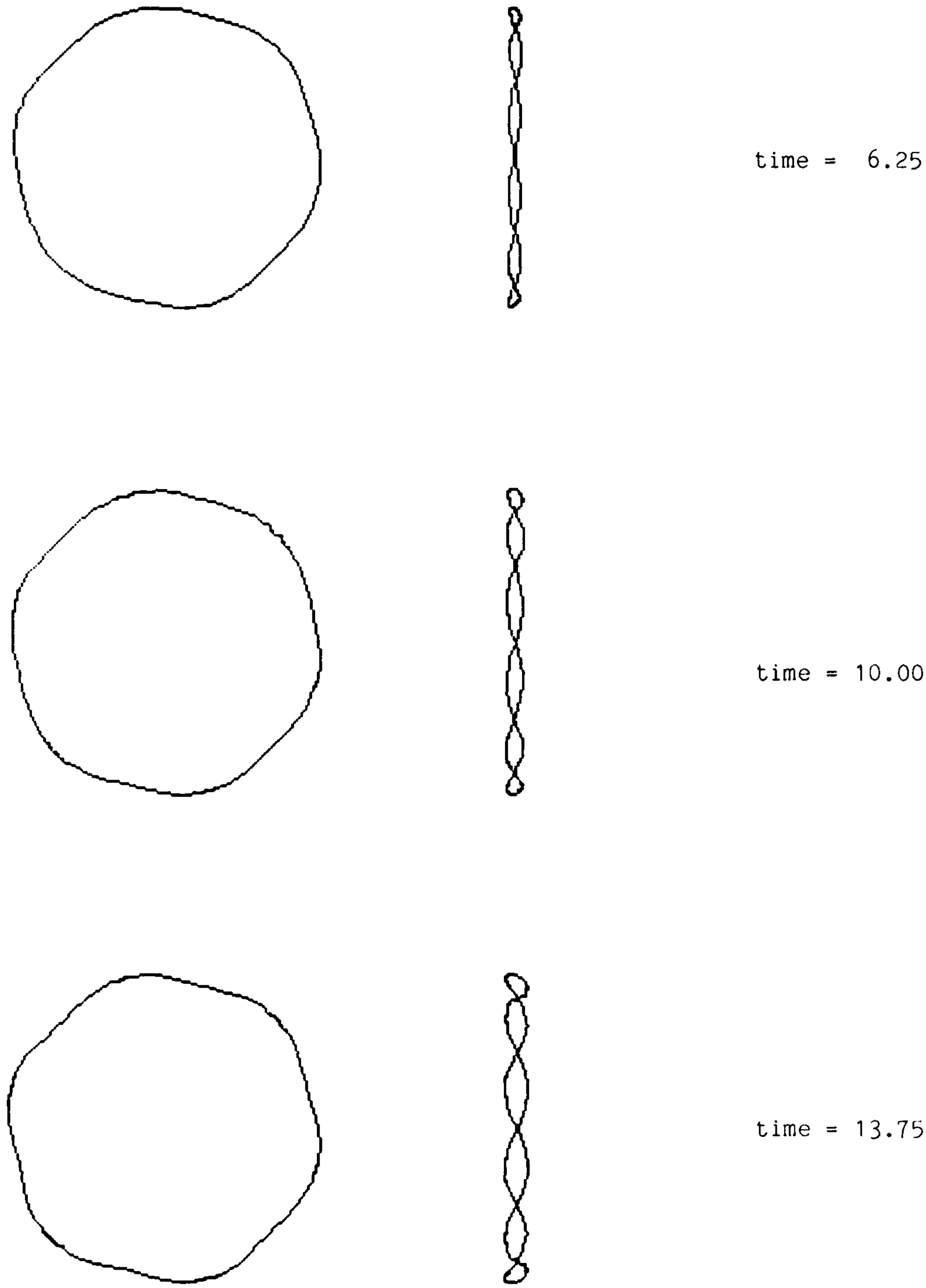


Figure 8 (a) Linear stages of development of instability waves around a vortex ring with core/radius = 0.25. The perturbation starts with six sine waves with amplitude 0.02, all in the radial direction and without streamwise component. Starting with different number of waves, the amplitude did not grow. Shown are three views of the ring at different time steps. Streamwise motion develops spontaneously. Within this stage, the amplitude grows exponentially, in accordance with the theory.

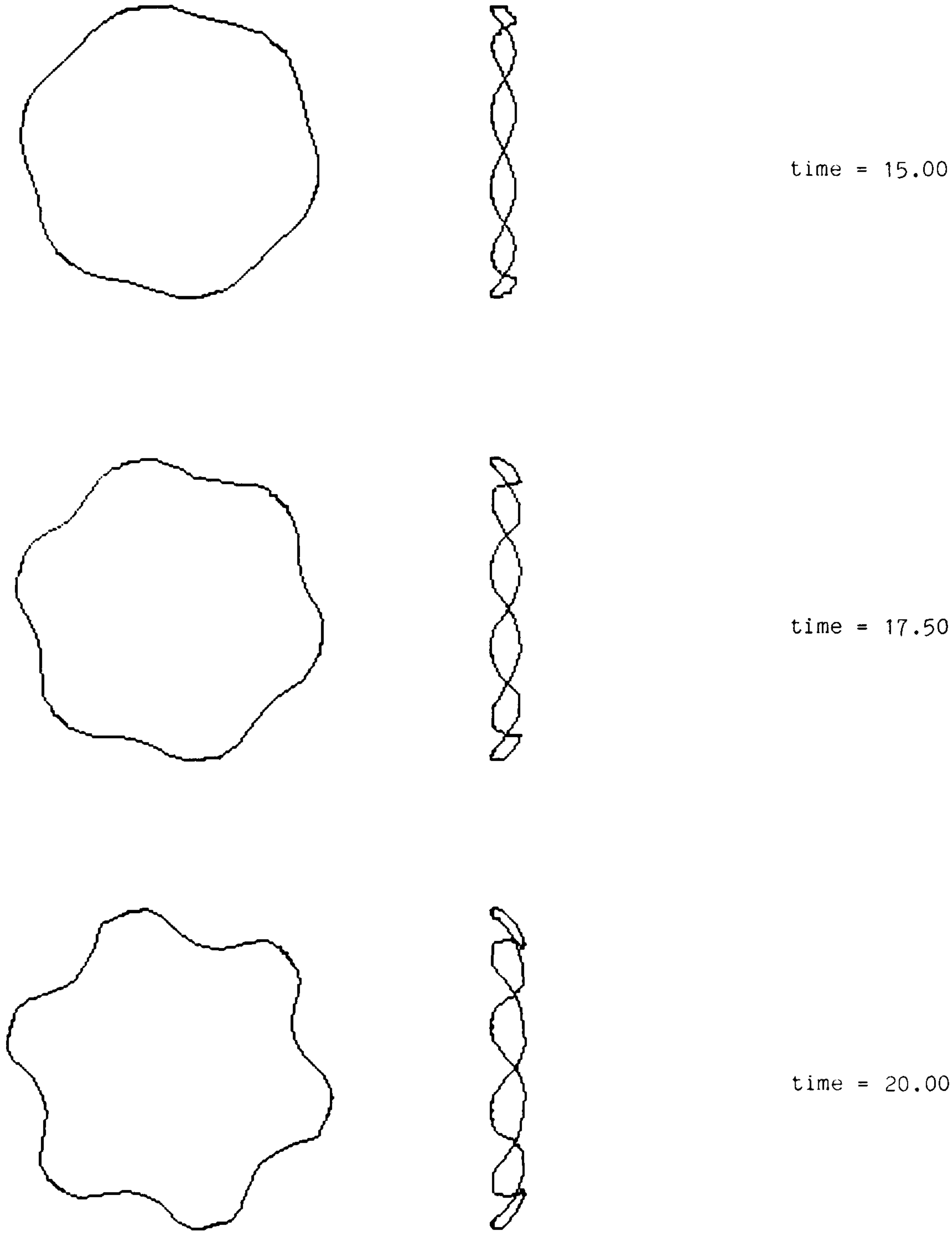


Figure 8 (b) Non linear development of instability wave around the ring. The ring experiences mild stretch in the streamwise direction and inverted U-shaped vortex lines start to appear permanently in the field. These inverted U-shaped lines bear a strong resemblance to the wiggles observed in the spanwise direction in a planar shear layer.

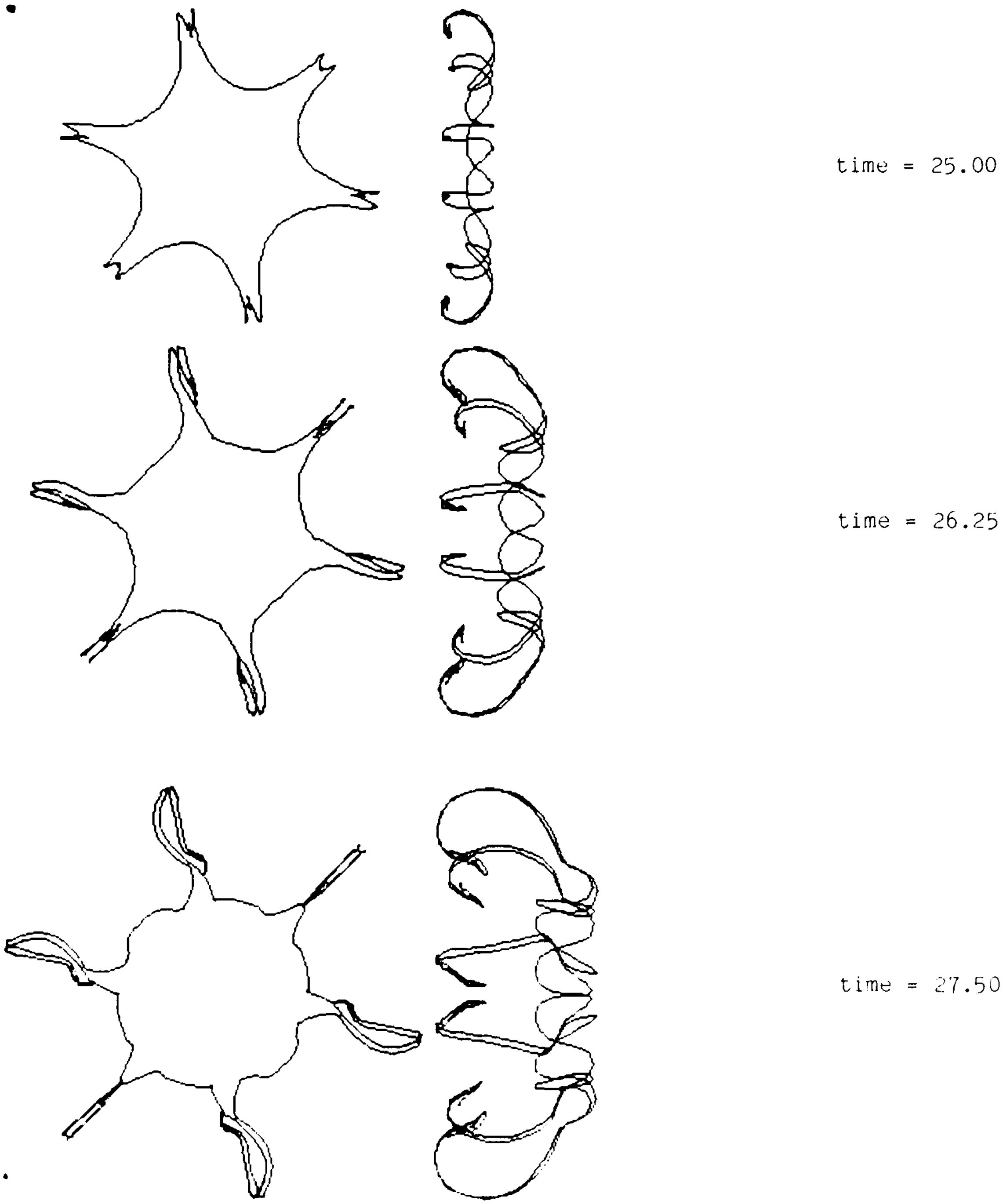


Figure 8 Later stages of development of the vortex ring, showing the the roll around of the stretched U-shaped lines into a "spider web" of strongly stretched vortex lines. The overall structure grows very rapidly and it is likely that the final stage would be a permanent transition to turbulence.

THESES PRODUCED DURING 1984-1986:

(1) Ng, Kenneth K., "Vortex Simulation of a Confined and Perturbed Shear Layer," M. Sc., January 1986.

(2) Gagnon, Yves, "Numerical Investigation of Recirculating Flow at Moderate Reynolds Numbers Using Vortex Methods," M. Sc., January 1986.

(3) Knio, Omar, "Low Mach Number Simulation of Combustion in Closed Chambers," M. Sc., January 1986.

PAPERS PUBLISHED DURING 1984-1986:

(1) Ghoniem, A.F. and Sethian, J.A., "Dynamics of recirculation in a turbulent flow; A computational investigation," AIAA-85-0146. The AIAA 23rd Aerospace Sciences Meeting, Reno, Nevada, 1985.

(2) Ghoniem, A.F., and Sethian, J.A., "Effect of Reynolds number on the structure of recirculating flows," accepted for publication at AIAA Journal (1986).

(3) Ghoniem, A.F., "Analysis of flame deformation in a turbulent field; effect of Reynolds number on the burning rate," AIAA-85-0140. The AIAA 23rd Aerospace Sciences Meeting, Reno, Nevada, 1985.

(4) Ghoniem, A.F., "Effect of large scale structures on tutbulent flame propagation," Combust. Flame, 64, 321-336 (1986).

(5) Ghoniem, A.F., "Computational methods in turbulent reacting flows," Invited three lecture series at The Seventh AMS-SIAM Summer Seminar in Applied Mathematics on Combustion and Chemical Reactors, Cornell University, July 1985. Lectures in Applied Mathematics, 24, pp. 199-265, 1986.

(6) Ng, K.K., and Ghoniem, A.F., "Numerical simulation of a confined shear layer," The 10th International Colloquium on the Dynamics of Explosions and Reactive Systems, August 4-9, 1985, Berkeley, CA. Dynamics of Reactive Systems, Part II, ed. by Bowen et al., 18-49 (1986).

(7) Ghoniem, A.F. and Gagnon, Y., "Numerical investigation of recirculating flow at moderate Reynolds numbers" AIAA-86-0370. The AIAA 24th Aerospace Sciences Meeting, Reno, Nevada, January 1986.

(8) Ghoniem, A.F., and Gagnon, Y. "Vortex simualtion of laminar recirculating flow," accepted for publication at J. Comput. Phys. (1986).

(9) Ghoniem, A.F.,and Ng, K.K. "Effect of harmonic modulation on rates of entrainment in a confined shear layer," AIAA-86-0056. The AIAA 24th Aerospace Sciences Meeting, Reno, Nevada, January 1986.

(10) Ghoniem, A.F., and Ng, K.K., "Numerical study of a forced shear layer," Accepted for publication at Phys. Fluids (1986).

(11) Ghoniem, A.F., and Knio, O.M., "Numerical Simulation of Flame Propagation in Constant Volume Chambers," Presented at The 21st Symposium (International) on Combustion, Munich, West Germany, August 1986. to appear in preceedings.

(12) Knio, O.M. and Ghoniem, A. F., "Modeling of combuation in confined chambers and the wrinkling of flames due to hydrodynamic instability," submitted for publication at Combust. Flame (1986).

(13) Sethian, J.A., and Ghoniem, A.F., "Validation of the vortex method," submitted for publication at J. Comput. Phys. (1986).

(14) Ghoniem, A.F., Knio, O.M., and Aly, H.F., "Three dimensional vortex simulation with application to axisymmetric shear layers," for presentation at the 25th Aerospace Sciences Meeting, Reno, Nevada, January 1987.

(15) Givi,P. and Ghoniem, A.F., "Vortex Scalar-element calculations of a diffusion flame," for presentation at the 25th Aerospace Sciences Meeting, Reno, Nevada, January 1987.

(16) Ghoniem, A.F., Heidarinejad, G., and Krichnan, A. "Vortex-Scalar Gradient Simualtion of a reacting shear layer," to be submitted for publication, J. Comput. Phys. (1986).

PRESENTATIONS DURING 1985-1986:

1. "Development and Applications of Vortex Methods: Aerodynamics and Combustion," NASA Lewis Research Center, Cleveland, Ohio, June 1984.

2. "Simulation of a Turbulent Flow in a Model Combustor," 1984 Technical Meeting, Eastern Section of the Combustion Institute, Clearwater Beach, FA, December 1984.

3. "Flame propagation and stability in engine chambers," Department of Energy sponsored program on "Lean Engine Efficiency," Ford Motor Company, May 1985.

4. "Numerical solution of a confined shear layer using vortex methods," The International Symposium on Computational Fluid Dynamics, Tokyo, Japan, September 1985.

5. "Vortex Simulation of Turbulent Reacting Flow," AFSOR/ONR Contractors Meeting on Turbulent Combustion, July 1985.

6. Ng, K. K. and Ghoniem, A. F., "Harmonic modulation of a confined shear layer," 1985 Technical Meeting of the Eastern Section of the Combustion Institute, Philadelphia, PA, November 1985.

7. Ghoniem, A. F. and Ng, K. K. "Numerical solution of a confined shear layer using vortex methods," The International Symposium on Computational Fluid Dynamics, Tokyo, Japan, September 1985.

8. "Application of Computational Methods in Turbulent Reacting Flow," University of North Carolina, October 1985.

8. "Vortex Simulation of Reacting Shear Flows," Army Research Office, Durham, North Carolina, October 1985.

9. The Pennsylvania State University, "Vortex Simulation of Reacting Shear Flow," November 1985.

10. Princeton Unversity, "Vortex Simulation of Reacting Shear Flow," December 1985.

11. University of California, Berkeley, "Computing Unsteady Flow Using Vortex Methods," Januray 1986.

12. Department of Energy Meeting on Homogeneous Charge Engines, University of California, Berkeley, April 1986.

13. Fourth Army Conference on Applied Mathematics and Computing, Cornell University, "Computing Unsteady Reacting Flow Using Vortex Methods," May 1986.

14. SIAM National Meeting, Boston, MA, July 1986, "Computational Methods in Combustion Theory".

15. Workshop on Computational Fluid Dynamics and Turbulent Reacting Flows, Institute of Mathematics and its Application, University of Minnesota, September 1986. "Vortex Simulation of Turbulent Reacting Flow".

INTERACTIONS DURING 1984-1986

1. Participated in DOD meeting on Topical Review on Mechanics, Aeronautics and Propulsion, National Academy of Sciences, February 5-6, 1985.

2. NASA Lewis Research Center, Combustion Fundamentals (Dr. C. John Marek) and Computational Fluid Mechanics (Dr. John Adamczyk), June 1984.

3. California Institute of Technology, Combustion Laboratory of Prof. E. Zukoski, to explore their experimental work on pressure oscillations in dump combustors and couple to our numerical studies, July 1985.

4. Army Research Office, Mathematical Sciences Division (Dr. J. Chandra) (to visit the Laboratory on October 4, 1985, and explore avenues for interactions).

5. Pennsylvania State University, Combustion Laboratory of Dr. Dominic Santavicca, to couple his experimental investigation on the effect of turbulence on flame propagation (supported by AFOSR) to our numerical simulation activities (to visit the Laboratory on November 6th).

6. Sandia National Laboratory, couple experimental work on flame structure (Dr. R. Green) and engine efficiency (Dr. F. Dyer) with our numerical simulation studies.

7. Columbia University, N.Y., Combustion Laboratory of Drs. R. Bill and R. Chevery, to couple their experimental work on stability of V-shaped flames and axi-symmetric shear layers to our numerical simulations (to visit during this academic year, 1985-1986).

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